A Survey on Contact Algorithms[1]

©Nicolai G. Bourago
Institute for Problems in Mechanics of Russian Academy of Sciences
prospect Vernadskogo 101, b1, 119529, Moscow
e-mail: burago@ipmnet.ru

Abstract

Most of natural and technological processes deal with interfacial boundaries between non-mixing medii of rigid, solid, liquid or gas nature. Present work aims to make a brief survey on contact algorithms developed worldwide during 40 recent years for calculation of contact, free and phase transition boundaries.

Introduction

A contact algorithm is a part of solution method, which is responsible for detection, tracking and calculation of contact, free or phase transition boundaries.

Contact algorithms can be separated into two major groups regarding the Lagrangian and Eulerian descriptions of continuum motion. In Lagrangian algorithms the nodes move with continuum, in Eulerian algorithms the nodes stay in place while the continuum moves through the stationary mesh or through Eulerian coordinate system. Non-Lagrangian algorithms deal with convection (advection) effect.

In both Lagrangian and Eulerian cases the contact (interfacial) boundaries can be treated explicitly (interface tracking algorithms) as a set of connected lagrangian surface nodes (markers) and cells, or implicitly by using some contact (interface) capturing techniques based on various implementations of continuous Lagrangian marker functions.

This classification is used as a skeleton for the survey. An additional review on special problem oriented contact algorithms, parallel processing and error analysis is also presented. The minimal set of references includes only some key and recent publications, which contain farther references. To save paper space instead of citation we submit multiple links to known related bibliography collections.

Compared to regular initial boundary value problem the statement of contact problems involves special boundary constraints, which govern the interface motion and possible singularities.

For classical contact problems the constraints express non-penetration (unilateral) condition, third Newton's law and law of surface friction. The normal contact condition prevents penetration of one body into another and the tangential slip represents frictional behavior of a contact surface. Extended physical formulation includes contact boundary conditions for thermal, electro-magnetic phenomena, diffusion and so on.

Additional contact relevant cases of free and phase transition boundaries are also under consideration here. A free surface is a Lagrangian interface between a dense media (liquid or solid) and a gas. Action of the gas is represented by external surface

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forces and its low density is neglected. At the free boundary a surface tension can take place. In contrast to contact and free boundaries the phase transition boundary is not Lagrangian and therefore in such a case problem formulation includes phase equilibrium relations, which define the non-Lagrangian interface motion.

A variety of possible formulations of differential, integral or variational type can be used. Among others the formulations in the form of variational inequalities serve to investigate the correctness of initial boundary value contact problems, reviews presented in (Lions, 1978; Kravchuk, 1997; Sadovskii, 1991, 1997, Kondaurov, 2002).

Numerical-analytical methods for contact problems, based on continuous approximations, include a great community of mathematical techniques such as asymptotic expansion, perturbation, singular integral equation, integral transformation methods and many others. Very fresh huge collections of reviews of such methods can be found in (Alexandrov, Vorovich (Eds.), 2001). In most cases numerical-analytical studies deal with simplified physically and geometrically formulations.

Current survey considers discrete numerical methods, which use grids or free nodes (Lagrangian particles) and are based on finite or quasi-finite approximations. Regarding the choice of problem settings and solution approximations the following general discrete techniques are typical: finite differences, finite volumes, finite elements, meshfree Galerkin, boundary elements. Compared to mentioned above numerical-analytical methods, the discrete methods are less restrictive in respect of problem formulations, which can be successfully implemented. Relative surveys can be found in (Hyman, 1984; Benson, 1992; Kothe et al., 1998; Fomin et al., 1999; Gil'manov, 2000; Osher, Tryggvason, 2001) and others, which are referred later.

1. Lagrangian interface tracking algorithms

Reviews of Lagrangian interface tracking algorithms can be found in (Oden, Martins, 1985; Kikuchi, Oden, 1986; Benson, 1992; Zhong, 1993; Fomin et al., 1999; Oishi, 1999; Diekman, 2000; Laursen, 2002).

In most of dynamic incremental (step by step in time) Lagrangian algorithms the contact boundaries are detected by the penetration of boundary nodes through alien boundary cells which may happen after predictor time step, which is calculated neglecting the contact.

The penetration takes place if a boundary cell is intersected with a nodal track. Alternative way of contact zone detection selects the boundary contacting pair "boundary node - alien boundary cell", if they are close enough to each other (much less than local spatial cell size).

On the corrector time step (or correction stage) the non-penetration constraints are taken into account. A lot of contact algorithms use Lagrange multiplier or penalty function techniques. The contact pressure (normal contact reaction force) plays the role of Lagrange multiplier for unilateral constraint. In case of penalty method the contact pressure is proportional to penetration (gap) in normal direction with large coefficient of proportionality (penalization of unilateral constraint). Description of algorithms and reviews can be found, for example, in (Hallquist, 1976, 1998; Fux, 1976; Hughes et al., 1976; Kikuchi, Oden, 1986; Bourago, 1987; Gulidov, Shabalin, 1987; Bourago, Kukudzhanov, 1988; Benson, 1992; Fomin et al., 1999;

Korobeinikov, 2000). See our extended survey (Bourago, Kukudzhanov, 2002a) for more complete script of publications and history of studies.

There are a number of alternative techniques of satisfaction the unilateral constraint. Simplified sliding algorithms of Wilkins family (Wilkins, 1964), local inelastic collision algorithms (Korneev, Shugalev, 1986) and many others. Transient hyperbolic contact problems can be effectively calculated with methods of characteristics (Kukudzhanov, 1985; Kondaurov, Petrov, Holodov, 1986) and with Godunov methods using solution of Riemann problem (Godunov et al., 1976; Bychek, Sadovskii, 1997; Sadovskii, 1998).

It should be mentioned that Lagrangian tracking of contact boundaries of solids and non wetting liquids needs a number of iterations because contact zone is unknown until the solution is obtained. It means that contact problems are nonlinear even in the cases of physically and geometrically linear problem formulation.

Detection of contact zone is a quite expensive procedure in the case of high resolution grids. In simplest contact pair search algorithm the penetration should be checked for each boundary node and cell. The amount of required calculations in such trivial contact search algorithm is proportional to second power of the boundary nodes number. Several enhanced contact search algorithms were developed to decrease required number of penetration checks. These improved contact search algorithms (Benson, 1992; Belytschko, Yeh, 1993; Oldenburg, Nilsson, 1994; Wang, Nakamashi, 1997; Petocz, Armero, 1998; Diekman et al., 2000) implement hierarchical cluster (group) search principle. Boundary nodes are united into groups of neighboring nodes. small groups are united into bigger groups. Search is organized as global selection of possible contact partners firstly among most big groups, then among smaller groups and so on. Final local search assumes selection of contact pairs ”node - surface element” within previously chosen smallest groups.

Contact search gap function algorithm (Hirota et al., 2001) stays apart and should be mentioned separately. The gap function is calculated for each grid node as a distance to the boundary. For boundary nodes it takes zero values. If grid overlapping happens then boundary node-intruder has two various values of gap function: first value is its own (zero) and second value corresponds to its position inside some grid cell. This second value is proportional to the distance to the boundary while local gap function anti-gradient defines the boundary external normal vector. The idea can be treated as a variant of the level set method (Sethian, 1999) for Lagrangian formulation.

Explicit Lagrangian contact algorithms are built also for tracking internal discontinuities, which imitate macro cracks. There are algorithms, which use local remeshing and introduce additional nodes in the parent cells containing damage interfacial boundary (Gridneva, Nemirovich-Danchenko, 1983; Larsson, Runesson, 1993, Fleming et al. 1997; Rashid, 1998; Daux et al., 2000; Dolbow et al., 2001; Duarte et al., 2001), and algorithms, which shrink damaged cells by shifting its nodes onto crossing interfacial surface (Gulidov et al., 1982; Kiselev, Kabak, 1990; Moes et al., 1999). Overview and description of such algorithms can be found in (Fomin et al., 1999).

2. Lagrangian capturing contact algorithms

Lagrangian capturing contact algorithms assume continuous solution at interfacial boundaries and use so called ideal contact model.

Simplest variant of "ideal contact" algorithm uses united Lagrangian grid in contacting bodies with common nodes at interfacial boundary. This technique gives acceptable solution for contact with no slip and connection/disconnection. Actually any grid based code can be easily used to model some cases of ideal contact.

In order to simulate possible contact discontinuities in a frame of united grid strategy the buffer layer algorithms are developed. These algorithms use predetermined intermediate buffer cells between contacting bodies (Chaboussi et al., 1973, Fridriksson, 1976; Michailovski, Mroz, 1976; Pozdnjakov, 1979; Desai et al., 1984; Nikishkov, Pashnin, 1986; Nikishkov, 1988) and many others. Review can be found in (Zernin et al. 2002). This technique simulates slip and connection/disconnection of contact boundaries properly for small deformations.

For large deformations and strongly variable contact zone buffer layer technique fails and its farther development leads to already considered general Lagrangian tracking algorithms with automated generation of contact pairs.

Internal contact discontinuities can appear if phase transitions take place. Interface capturing techniques for such processes are based on unified constitutive equations, which describe the phase transition and phase behavior. Good example is given by numerical implementations of continuous damage constitution models, which simulate growing macro cracks and strain localization in solids (Maenchen, Sack, 1964; Lemaitre, 1996; Tomita, 1994; Kukudzhanov et al., 1995; Benaroya, 1996; Bourago et al., 2000; Bourago, Kukudzhanov, 2002a).

3. Eulerian interface tracking algorithms

In many problems, such as problems with opened boundaries, with extremely large deformations or with variable topological properties, Lagrangian description of motion becomes not comfortable while Eulerian algorithms appear more suitable. In Eulerian contact algorithms solution is continuous and possible interfacial singularities (shocks) are simulated as high gradient narrow zones.

Eulerian interface tracking algorithms use Lagrangian particles or markers to track interfacial boundaries. To implement dynamic boundary conditions such algorithms connect boundary markers (particles) into Lagrangian cells to calculate local interfacial vector basis and curvature. Motion of markers is calculated using material velocity definition. Variants of such algorithms are presented by (Harlow, 1964; Noh, 1964; Welch et al. 1965; Nickols, 1973) for fluids and by (Kalmykov, Kukudzhanov, 1992; Fomin et al., 1999) for elastic plastic solids. Coordinates are the only characteristics of markers while particles transfer mass, momentum, energy and other material properties and therefore with particles there are no difficulties with convective terms. Instead there are difficulties with lack of particles and markers in zones of strong extension.

4. Eulerian interface capturing algorithms

Discrete marker techniques strike with difficulties in cases when dynamic boundary conditions should be taken into account and accurate calculation of normal, tangential vectors and curvature of the interface is required. These difficulties are conjugated with necessity to track the boundary lagrangian markers (particles) and cells in cases of fragmentation or merging boundary surfaces or large boundary distortions.

To overcome these difficulties the concept of continuous Lagrangian marker functions is used. Any continuous Lagrangian marker function is subjected to transport equation and keeps constant value along Lagrangian tracks. Interface boundary is tracked as contour surface, which responds to definite level of marker function. Local surface basis vectors and curvature are defined by using the derivatives of marker function.

Various implementations of continuous marker concept can be found in (Erlich, 1958; Oleinik, 1960; Samarskii, Moiseenko, 1965; Belotserkovskii, Davydov, 1982; Rvachev et al., 1980, 1995; Hirt, Nickols, 1981; Thompson, 1986; Brackbill et al., 1988; Sussmen et al., 1999; Sethian, 1999; Enright et al., 2002, Osher, Fedkiv, 2002; Benson, 2002). Osher and Sethian have chosen distance to interface as a continuous marker in their level set method. In contrast to many relevant methods which use Heaviside marker functions there are no trouble with interfacial diffusion. In most Eulerian algorithms conservation laws are violated near interfacial boundaries, so a control and special corrections are needed.

5. Adaptive grids and shock capturing

It was mentioned that interfacial boundaries are zones of high gradients, therefore shock capturing techniques and adaptive grid methods can be used to improve an accuracy of numerical implementations of contact algorithms.

Reviews of shock capturing techniques presented in most of modern books on Computational Fluid Dynamics, for instance, very fresh survey can be found in (Kulikovskii, Pogorelov, Semenov, 2001).

Reviews on adaptive grid refinement and adaptive moving grid techniques can be found in handbook on grid generation (Tompson, Soni, Wheatherill (Eds.), 2000) and in recent monographs (Carey, 1997; Ivanenko, 1997,1999; Liseikin, 1999; Gil'manov, 2000). See also reviews in (Li, Bettess, 1997; Mikolajczak et al., 2000).

6. Meshless methods

To avoid problems induced by Lagrangian grid distortions and simultaneously to stay in the frame of Lagrangian approach Belytschko et al. (1994, 1996) proposed the Element Free Galerkin (EFG) method with an accurate numerical integration and accurate treatment of essential boundary conditions. Liu et al., (1996) developed the relevant Reproducing Kernel Particle Method (RKPM), which was further extended to highly nonlinear hyperelasticity by Chen et al. (2001).

It should be mentioned that first attempts to create meshless Lagrangian algorithms (free Lagrange methods) have been made in (Pasta, Ulam, 1959; Ulam, 1964; Djachenko, 1967, 1973; Glagoleva et al., 1972; Anuchina et al., 1980; Monaghan, 1982). Review presented in (Li, Liu, 2002).

The intention to avoid grid generation problems has been implemented also in boundary element (integral) contact algorithms, reviewed in (Goldshtein, Spector, 1986; Aliabadi,1997; Eck, Wedland, 1999). In case of nonlinear formulation boundary element method requires external iterations and volume integral calculations. This results in the loss of advantage of using only surface grid and creates additional difficulties due to bad convergence of external iterations.

7. Vectorization and parallelization of contact algorithms

Vectorization of Lagrangian contact algorithms is not effective because they operate with vectors of much smaller length compared to the total grid node number. Vectorization of contact algorithms considered in (Hallquist, 1976,1998; Bourago, Kukudzhanov, 1988; Ginberg, Katnik, 1989).

Parallelization of Lagrangian contact algorithms is reviewed in (Oishi, 1999; Brown et al., 2000). Highest achievement in efficiency of parallelization is described in (Attaway et al., 2001).

8. Specialized contact algorithms.

Contact friction is usually simulated in accordance with 1) modified Coulomb friction law (Michailovski, Mroz, 1985; Wriggers et al., 1990) which takes into account dependence of friction forces on contact pressure, displacement jump and material properties of contacting medii, and 2) dynamic friction law (Oden, Martins, 1985), which takes into account dependence of friction forces on contact velocity jump. Review of contact friction laws can be found in (Kalker, 1990; Bhushan, 1996; Gorjacheva, 1998).

Contact algorithms are used as a variant of grid generation strategy to implement of ideal contact conditions on non-matching interfacial meshes at the subdomain fictitious boundaries in cases of complex geometry. Such policy provides continuous solution without grid adjustment at the artificial interfaces (Bazhenov et al., 1984, 1995; Park et al., 2000; Felippa et al., 2001).

Many practical problems deal with multiple interfacial boundaries. Examples are layered and block structured medii, composites, cavitation and bubbles in fluid flows, polycrystal growth and many others. Explicit tracking techniques fail to solve such problems even if high performance supercomputers are used. Mentioned above Lagrangian and Eulerian interface capturing techniques can be very useful for such problems, see for instance multiphase contact algorithms in (Udaykumar et al., 1999; Kunugi, 2002).

With further increase of a number of interfacial boundaries another policy becomes more useful and efficient: averaging constitutive models. Examples of such models are given by theories of layered and block medii (Nikitin, 1989), consolidation (Riedel, Sun, 1992), damage (Lemaitre, 1996; Bourago et al., 2000; Kondaurov, 2001), phase transitions (Kondaurov, 2002).

Shape design optimization contact algorithms are used to prevent appearance of non desirable contact reaction peaks, which can effect the functionality of technical devices. Linear programming techniques applied in (Conry, Seireg 1971; Haug, Kwak, 1978), nonlinear programming finite element algorithms presented in (Cheng et al., 1988; Belegundu, Chandrupatla, 1980; Clarke, 1983; Tada, Nishihara, 1993; Park, Anderson, 1995; Fancello, 1995; Xie, Stiven, 1997;). Fresh reviews can be found in (Seireg, Rodriguez, 1997; Chen et al., 2001).

Contact algorithms for animation use kinematic approaches. In these methods, the impenetrability constraint is satisfied by heuristic techniques, often requiring extensive and boring user control and interaction to produce the desired effects of satisfactory quality. Simple contact tracking algorithms reviewed in(Bechmann, 1994; Lewis et al., 2000) do not follow physical laws.

Contact algorithms for biomedical applications present farther motion towards mechanics. These algorithms serve to model the processes and results of surgery operations. Reviews of such algorithms, which already take mechanical laws into account, are made in (Gourret et al., 1989; Hirota et al., 2001)

Here we give links to bibliography collections on contact algorithms for: geomechanics (Moresi, 2002), free and moving boundaries for Hele-Shaw and Stokes flow (Gillow, Howison, 2002), moving-free boundary for heat-diffusion and Stefan problem (Tarzia, 1988; Florian, Rasmussen, 1989; Shyy et al. 2001), cavitation problems (Wikstrom, 2000), cloth behavior modeling (Baraff, Witkin, 1998).

9. Error estimate, testing and critical analysis of contact algorithms

All contact algorithms give only approximate solutions. Not so many works are devoted to error estimates, testing, comparison and critical analysis of contact algorithms. Here is the script of such studies found: (Lee et al., 1991; Lee, Oden, 1993a, 1993b; 1994; Cvetkova, 1995; Christiansen et al., 1998; Sharif, Wiberg, 2001).

Comparison of different algorithms is not simple because results depend on quality of code and on undocumented features of contact algorithms. Unfortunately, quite rare studies compare codes which are made by one and the same group of scientists by using one and the same computing "kitchen", while exactly that kind of comparison can give most valuable and definite results. It is so because very often some negligible detail of the algorithm, which never is mentioned in papers or reports, can play important role in success of the modeling. Mostly it happens because each algorithm has a great number of consistent parts and at the same time there is no unique way of their implementation.

A good example of comparison analysis of contact algorithms is presented in (Rider, Kothe, 1995) on numerical modeling of two-phase flow. Four different test problems are used for evaluation of interface tracking methods: simple translation, solid body rotation, a single vortex and a complex deformation field. The methods studied are: variant of marker particle method (Brackbill et al., 1988), variant of volume-of-fluid (VOF) method (Kothe, Rider, 1994), level set method (Sussman et al., 1999) and monotone slope-limited shock capturing technique (Colella, Woodward, 1984).

By the quality of results the methods are placed in the above order. The only method that remained robust was the marker particle method. After analysis of possible improvements the new method was created: Hybrid Particle Level Set Method (HPLS, see Enright et al., 2002). Authors claim the it accumulates the best features of discrete and continuous markers and successfully passes all mentioned tests.

Conclusive remarks

Big number of various contact algorithms show that they are not ideal and each has its own advantages and drawbacks. Anyone should be very careful in judgements about quality of existing contact algorithms and their ability to solve a variety of problems. Symptoms of overestimating have been very well illustrated by N. Johnson (1996). He collected a number of following rather typical advertising declarations, which everyone can hear rather often from CFD code developers:

"It will solve your problem without modifications."

"The manual has everything you need to run the code."

"Standardized graphics output, compatible with third party post-processors."

"Minimal learning curve."

"Executable on all machines with no modifications"

"Robust and accurate."

"All physics are compatible."

"User friendly."

"There are no more bugs in the code, only undocumented features."

"You can run the code without the manual."

"The technique was first developed here."

No comments required.

For more information on contact algorithms read our extended version of current survey (Bourago, Kukudzhanov, 2002), which contains historical issues and more detailed analysis of about 600 works on contact algorithms.

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